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Progress in Mix Modeling

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We have identified the Cranfill multifluid turbulence model (Cranfill, 1992) as a starting point for development of subgrid models of instability, turbulent and mixing processes. We have differenced the closed system of equations in conservation form, and coded them in the object-oriented hydrodynamics code FLAG, which is to be used as a testbed for such models.

Introduction

There are a number of physics problems in which the mixing of fluids under acceleration involves multiple processes and flow regimes, including but not limited to fully-developed turbulence. For instance, such "laminar mixing" processes as Rayleigh-Taylor, Richtmyer-Meshkov and Kelvin-Helmholtz instabilities may be significant both in determining the manner of the onset of turbulence and as mixing processes in their own right. Supernovae, ICF targets, and many types of combustion, turbomachinery and explosion problems are examples of systems which can only be understood by including both turbulent and laminar mixing phenomena.

Since laminar mixing processes are by definition not turbulent, and due to other characteristics they possess such as anisotropy and low entropy (as shown by the possibility of demixing; see Smeeton and Youngs, 1988), we should not expect to predict their behavior with subgrid models of isotropic turbulence, such as the widely used two-equation models. In order to incorporate information about anisotropy and for other reasons, it is attractive to marry the equations of multifluid hydrodynamics with a turbulence model. This approach has been explored by several workers in the field (see for instance Besnard et al., 1989; Youngs, 1989; and Cranfill, 1991). We find the multifluid approach particularly attractive for modeling the laminar mixing processes because, by allowing each constituent to have its own velocity field, we can model segregation of materials, anisotropy, partial reversibility (demixing) and mass transport (mix) by streaming, without explicitly resolving the subgrid-scale structure of the interface and mixing region.

We are developing mix models of the hybrid (multifluid–turbulence) type, and testing them in a research code. As a theoretical starting point for this work we have adopted Cranfill's (1992) improved model. This is a closed, internally consistent set of equations which models both turbulence and the mutual interpenetration of fluids. We have differenced the Cranfill model and implemented it in the object-oriented Lagrange hydrodynamics code FLAG. We intend to develop new models as variants of or additions to the Cranfill model, testing them in the code.

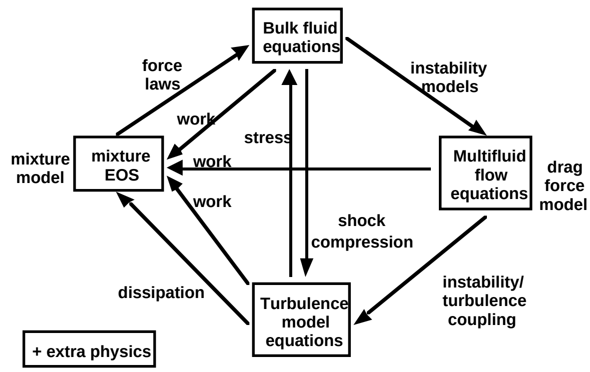

Figure 1. Schematic diagram of the Cranfill model. Unboxed text identifies physical processes that are or could be accounted for in the model. "Extra physics" refers to coupling between fluid dynamics and other physical processes that may be acting, e. g., reaction energy in a combustion problem. Our research objective is to examine the adequacy of the model to describe all these processes, and improve it where appropriate and feasible.

The Cranfill multifluid turbulence model

Model philosophy

Cranfill (1992) decomposed the fluid properties into three parts: the mean flow, described by Navier-Stokes equations; "ordered convective" turbulence, modeled by his multifluid interpenetration equations; and "disordered diffusive" turbulence, which is described by a two-equation (k-ℓ) turbulence model. The "ordered convective" turbulence is what we have called "laminar mix," that is, flow which is disordered but not well mixed, so that the different fluids present have different mean velocities. An example of this is the early stage of Rayleigh-Taylor instability, in which well-defined bubbles of one fluid and spikes of the other are moving past each other. "Disordered diffusive" turbulence is what we might call fully-developed turbulence; the system is well mixed, so that all materials have essentially the same mean velocity and demixing is not possible under the action of long-wavelength driving forces. In such a mixture the motions of different fluids are so strongly coupled that it is a good approximation to regard them all as being equally turbulent (in a sense which is made clear in the model details). For this reason, a single turbulent energy field k is applied to the entire system, rather than keeping a distinct turbulent field for each material.

The model equations are derived by Favre averaging the fluid equations and using modeling assumptions to close the system. The rigor of the derivation from fluid equations guarantees conservation and other desirable constraints, which we will preserve in our variant models. On the other hand, the modeling assumptions can presumably be improved without violating important physical principles. We will develop and test improved models of individual phenomena by replacing some of the terms or equations which embody those assumptions.

Model equations

For full details of the model equations and their derivation, the reader is referred to Cranfill's (1992) report.

In our initial form of the coded model, we have omitted terms depending on molecular viscosity η and thermal conductivity κ. We have, however, kept the dissipation of disordered turbulence ε_d, in conformity with common practice in turbulence modeling. In conservation form, the differential equations of the model can be expressed as follows:

Bulk fluid equations.

$$\frac{d}{dt}(M) = 0 \tag{1}$$

$$\frac{d}{dt}\vec{p} = \vec{F}_o + \vec{F}_d + \vec{F}_P \tag{2}$$

$$\begin{aligned}\frac{d}{dt} I = &-Flux_o^I - Flux_d^I - Work(P,\vec{u}) \\ &-Work(P,\vec{w}) + Dissip(d \to i)\end{aligned} \tag{3}$$

In these equations, M and $\vec{p}$ are the total mass and momentum in a control volume; $\vec{F}_o$, $\vec{F}_d$ and $\vec{F}_P$ are the forces on that volume due to ordered and disordered turbulence and pressure; $Flux_o^I$ and $Flux_d^I$ are energy fluxes into the control volume due to ordered and disordered turbulence; $\vec{u}$ is the mass-weighted mean velocity; $\vec{w}$ is the drift velocity, defined as the difference between the volume-weighted mean velocity and $\vec{u}$; $Work(P,\vec{u})$ and $Work(P,\vec{w})$ are the pressure work done by the fluid corresponding to $\vec{u}$ and $\vec{w}$; and $Dissip(d \to i)$ is the rate of energy dissipation from disordered turbulent energy to internal energy. The convective or Lagrangian derivative is represented by the notation $d/dt \equiv \partial/\partial t + \vec{u}\cdot\vec{\nabla}$.

Ordered convective fluid properties.

$$\frac{d}{dt} M_j = -Flux_o^{M_j} \tag{4}$$

$$\begin{aligned}\frac{d}{dt}\vec{p}_j = &\vec{F}_{oj} + \vec{F}_{dj} - x_j\left(\vec{F}_o + \vec{F}_d\right) + \left(f_j - x_j\right)\vec{F}_P \\ &+ \vec{F}_{drag,j} - \vec{p}_j \cdot \vec{\nabla}\vec{u}\end{aligned} \tag{5}$$

Here M_j is the mass belonging to material j in the control volume; $\vec{p}_j \equiv M_j \vec{w}_j$ is the drift momentum of j, where the material drift velocity $\vec{w}_j$ is defined as its volume-weighted mean velocity minus $\vec{u}$; $\vec{F}_{oj}$, $\vec{F}_{dj}$ and $\vec{F}_{drag,j}$ are the forces on j due to ordered and disordered turbulence and intermaterial drag; and f_j and x_j are the volume and mass fractions of material j.

Disordered diffusive fluid properties.

$$\begin{aligned}\frac{d}{dt} K_d = &-Flux_o^{K_d} - Flux_d^{K_d} \\ &-Work(\boldsymbol{R}_d,\vec{u}) - Work(\boldsymbol{R}_d,\vec{w}) \\ &+Dissip(o \to d) - Dissip(d \to i)\end{aligned} \tag{6}$$

$$\begin{aligned}\frac{d}{dt} L = &-Flux_o^L - Flux_d^L \\ &-C_{\ell o} L \frac{1}{V}\frac{dV}{dt} - \tfrac{3}{2}\frac{C_{\ell o}}{C_\omega}\frac{\omega}{L}\end{aligned} \tag{7}$$

These are the new variables in this two-equation turbulence model : K_d and L are the energy and characteristic length scale of disordered diffusive turbulent flow in the control volume; $Flux_o^{K_d}$, $Flux_d^{K_d}$, $Flux_o^L$ and $Flux_d^L$ are the fluxes of those quantities into the control volume due to ordered and disordered turbulent flows; $Work(\boldsymbol{R}_d,\vec{u})$ and $Work(\boldsymbol{R}_d,\vec{w})$ are work done by the fluid due to the disordered turbulent Reynolds stress $\boldsymbol{R}_d$; $Dissip(o \to d)$ is the rate of energy dissipation from ordered to disordered turbulent energy; V is the volume of the control volume; ω is a characteristic rate for the intermaterial drag forces, modeled as a function of K_o, K_d and L; and $C_{\ell o}$ and C_ω are adjustable dimensionless constants.

Model implementation in the FLAG code

In order to be useful as a testbed for putative subgrid mix models, the research code should satisfy several important criteria. It must be flexible enough not to seriously constrain the physics; it should be easy to modify quickly and reliably; and it should use data structures and routines which support the description of mixtures and multifluid flow. It should also provide as many as possible of the utilities and physics capabilities needed to build mixing models, such as mixed EOS treatments, advection, accurate hydro and arbitrary dimensionality (to enable us to test the same models and coding in one, two and three dimensions).

We have experience in the installation of a multifluid model into a mature code which did not have all these characteristics. In particular, the original data structures, in which most physics variables were centered on a mesh cell, had to be replaced with a scheme in which many variables are centered on a material component of a cell. This necessitated inserting a new data structure between the cells and their elemental constituents, so that each zone contained one or more materials, and each material contained one or more constituents. The result is that hundreds of routines and tens of thousands of lines of code are affected. This upgrade will be a major code revision by the time it is complete.

By contrast, the FLAG code (Burton, 1992b) is well-suited to this project. Its object-oriented architecture and hierarchical database make it extremely modular and flexible. It is easy to modify quickly and reliably, and its data structures and routines were designed from the outset to describe mixtures of materials.

FLAG contains an accurate hydro package (Burton, 1990a; Burton, 1990b; Burton, 1992a; Burton, 1994a; Burton, 1994b), and pressure– and temperature–equilibrium routines for the effective EOS of mixtures. It runs in arbitrary dimensionality. An advection capability is being developed.

For all of these reasons, we identified FLAG as the most suitable research code for this project. To begin with, we differenced the Cranfill equations in conservation form. Then, in spite of our lack of direct substantial experience with FLAG, we were able to code the Cranfill model in three weeks' time. The new package is modular, so that we altered fewer than 50 lines of existing source files (subroutines and dictionaries). By utilizing and creating polymorphic routines for geometry-dependent functions, we wrote purely dimensionality-independent physics routines; the new package will run in one, two or three dimensions.

We made extensive use of pre-existing reusable functions and data types, but we also extended the code's object-oriented structure by introducing new reusable types, classes and functions. For instance, a mix calculation will use multiple objects belonging to the Multifluid class and one object of the Turbulence class, corresponding to the multiple fluids and single turbulent energy field of the Cranfill model. The new classes have their own forms of preexisting polymorphic functions such as FORCE and WORK, and new ones such as MIX. The online user manual (html files) was automatically updated to include the new classes, functions and variables. Their definitions and documentation are specified in dictionary files; a typical entry (abbreviated slightly for pedagogical reasons) is given in Figure 2.

```
class( Turbulence "Disordered turbulence as a material"
(from (MatBasic)
 proc (CleanState ConstitTb
       FORCE      undefined
       ETrans     ETransTb
       MIX        MixTb
       RATE       none
       WORK       WorkTb    )
 var (
 $ Constants
  comega   "Constant C sub omega"               ( TYPE r_scal INIT InitComega)
 $ Phases
  hkd      "Disordered turbulent energy k d"     ( TYPE r_H    INIT 0. )
  hko      "Ordered turbulent energy k o"        ( TYPE r_H    INIT 0. )
  hl       "Turbulent length l"                  ( TYPE r_H    INIT 0. )
  hepsd    "Disordered dissip. rate epsilon d"   ( TYPE r_H    INIT 0. )
  hreyo    "Ordered Reynolds stress R o"         ( TYPE r_K6H  INIT 0. )
  hreyd    "Disordered Reynolds stress R d"      ( TYPE r_K6H  INIT 0. )
 $ Material nodes
  ow       "Vol.-weighted mean drift velocity w" ( TYPE r_Ko   INIT 0. )
  oso      "Ordered turb. int. energy flux s o"  ( TYPE r_Ko   INIT 0. )
  osd      "Disord. turb. int. energy flux s d"  ( TYPE r_Ko   INIT 0. )
  odd      "Disord. turb. diffusion tensor D d"  ( TYPE r_K6o  INIT 0. )
 )))
```

Figure 2. Dictionary file entry defining Turbulence class (abbreviated).

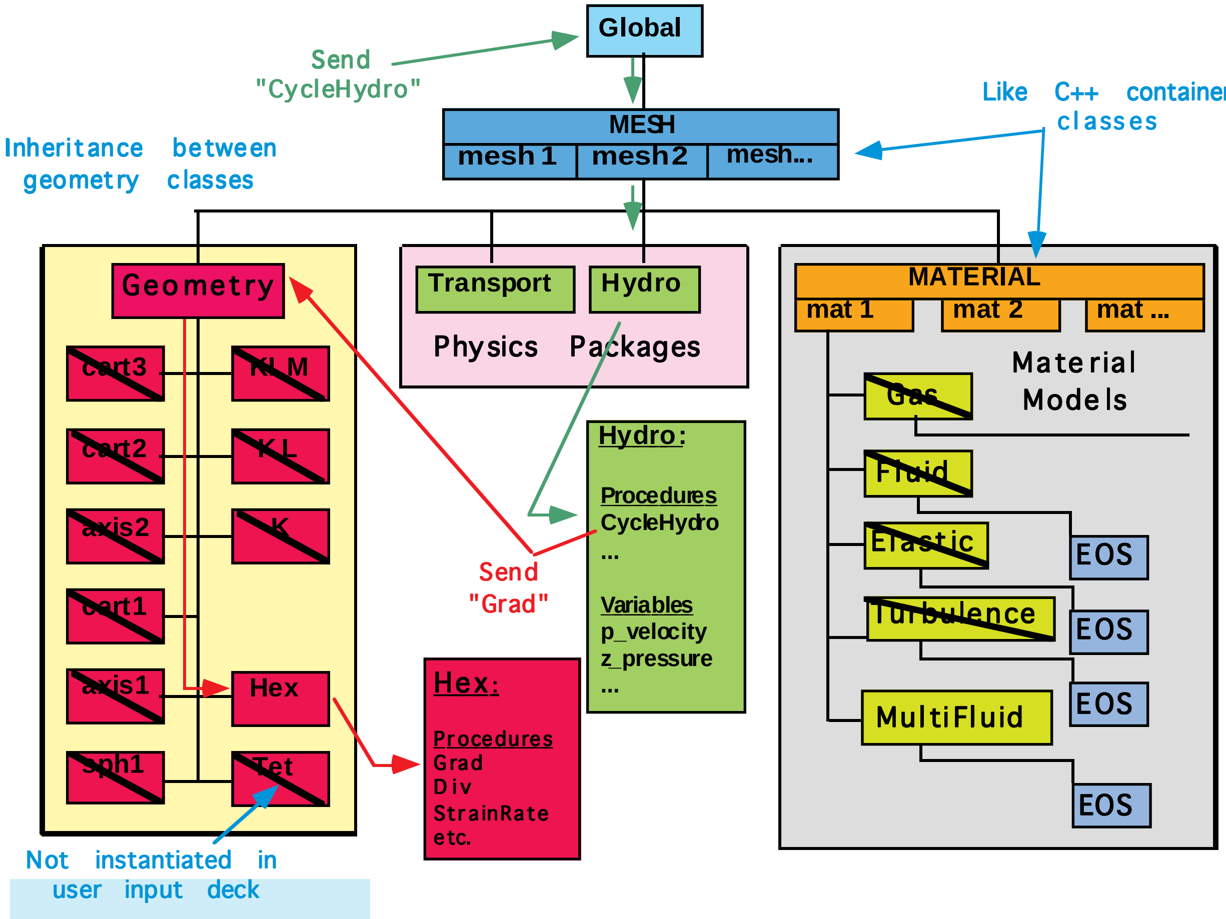

Figure 3. Schematic diagram of message passing among nodes in a representative portion of FLAG's hierarchical database; see text for details.

Physics and other data in FLAG are arranged in a hierarchical database. (See Figure 3.) This allows the code to use multiple instantiations of the same variable, defining non-overlapping scopes for each copy. (As an example, the same EOS parameters can have different values, or even different variable lists and array shapes, in different materials.) In a typical routine, most of the data used (besides temporaries) is from a single node of the hierarchy, but data above that node can also be accessed. A routine can also broadcast messages—effectively polymorphic function calls—to a subtree of the hierarchy. For instance, when the message "CycleHydro" is broadcast, the hydro package responds by executing its cycling function. The other physics packages do not, because they have no polymorphic form of the "CycleHydro" function. When the hydro package broadcasts "Grad" from the Geometry node, only that mesh type[1] responds which is instantiated in the problem, and the appropriate gradient routine is executed. The hydro package also broadcasts a "FORCE" message from the Mesh node, to which each instantiated material responds with the appropriate subroutine call. In this case, the Turbulence and Multifluid nodes in the hierarchy calculate all the pressure and turbulent forces which appear in equations (2) and (5) above, in such a way that each is automatically applied to the proper material(s).

[1]In principle, there can be multiple meshes in a problem, in which case all those instantiated will respond by calling the appropriate routine.

Research plans

This code package is one of the initial tasks in an ambitious, multi-year research project involving several researchers. We intend to assimilate information from theory, experiments and direct numerical simulation (DNS) to understand and characterize the numerous phenomena which are important in mixing processes. These include, for example, Rayleigh-Taylor, Richtmyer-Meshkov and Kelvin-Helmholtz instabilities, interactions between turbulence and shocks, other compressibility effects, transition to turbulence, loss of memory of initial conditions and coupling to other physics processes. While a perfectly general subgrid model is desirable, it may be more practical to devise different theoretical or phenomenological models for different flow regimes, with well-behaved transitions between regimes. This has been done in other complicated fluid dynamics problems; for example, see Figure 4 for an example (Yadigaroglu, 1995) from a commercial multiphase flow code (RELAP5/MOD2).

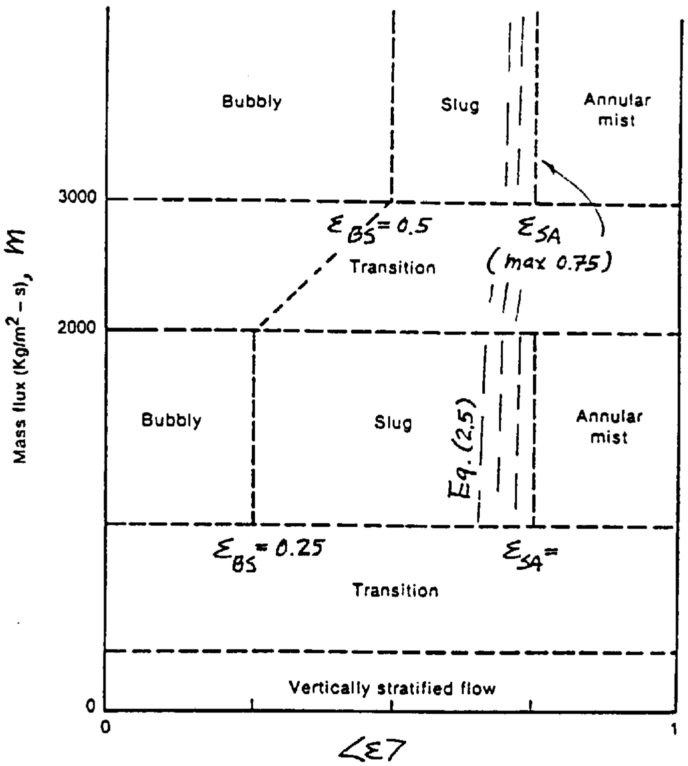

Figure 4. Flow regime selection logic used in RELAP5/MOD2 for vertical flow.

In any case, proposed models will be tested in the FLAG mix package, and iterated toward the most successful forms. We welcome the interest and participation of friendly users, as well as theoretical ideas and experimental and DNS data to motivate new and better subgrid models.

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